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Heat of Formation of OBrO: An Experimental Photoionization Study

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The potential importance of OBrO in atmospheric chemistry has been suggested recently. Although there appear to be no experimental measurements of $\Delta H(\text{OBrO})$, estimated values range from 70 to 152 kJ/mol [Chase, M. W. J. Phys. Chem. Ref. Data, 1996,25, 1069; *ibid*, 1297]. In the present investigation, the appearance energy (AE) of BrO^+ from OBrO was measured by employing a discharge flow-photoionization mass spectrometer that is operated at beamline U-11 (National Synchrotron Light Source/ Brookhaven National Lab). The heat of formation was derived from the AE result and the ionization energy of OBrO [IE=10.29 eV, Thorn et al., J. Phys. Chem. A 1999, 103, 8384]. The AE experiments yield a threshold at about 98.7 nm that gives, in turn, a value for $\Delta H(\text{OBrO})$ of 180 ± 10 kJ/mol. The difference with the estimated values mentioned above and the concomitant implications for the atmospheric reactions of OBrO will be discussed.

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